'Grand Challenges' in Correlated Electron Physics

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Outline

- 'New' quantal phases
- Controlling (and measuring) the quantum
- Strong fluctuations and physical properties
- The 'Kotliar revolution': spectral function not particle.
- Life at the edge: surfaces and interfaces of correlated electron systems



In the rest of this talk:

Recent work, which seems to raise important questions



Three Catch-Phrases

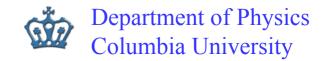
"What a Difference Between a Truth That Is Glimpsed and a Truth That Is Demonstrated"

Unnamed "18 Century French Admirer of Newton"

"That [which is] now proved was once only imagined"

William Blake

It's all about materials



Condensed Matter Physics: CANONICAL QUESTIONS

- What is the phase?
- What are the linear response functions?
- What are the (weakly interacting) particles in terms of which one understands linear response?



Insulating Magnets

Conventional Picture

Alternative (Anderson)

Phases: Long Range Ordered

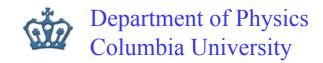
Phase: spin liquid

Response function: $M(q, \bullet)$

Response: Topological

Particles: Spin Waves

'Particles'--spinons



Numerical Evidence for Spin Liquid

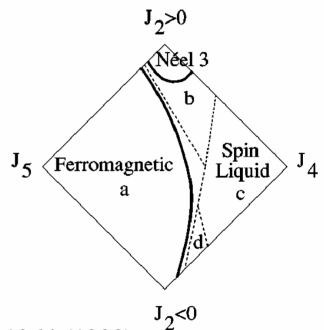
Ring Exchange Hamiltonian

$$H = J_{2} \sum_{\bullet \bullet} P_{2} - J_{3} \sum_{\bullet} (P_{3} + P_{3}^{-1})$$

$$+J_{4} \sum_{\bullet \bullet} (P_{4} + P_{4}^{-1}) - J_{5} \sum_{\bullet} (P_{5} + P_{5}^{-1})$$

$$+J_{6} \sum_{\bullet} (P_{6} + P_{6}^{-1})$$

Phase Diagram (numerics: 36 spins)



Misguich, Lhuillier, Bernu, Waldtmann, PRB60 1064 (1999)
See also Moessner and Sondhi, PRL 86 1881 (2001) (dimer model)

But—does it exist in real systems?



But in Real Systems???

No long ranged order—need to look for

- •Ground state degeneracy (on a torus
- Edge States (if gapped spin liquid)



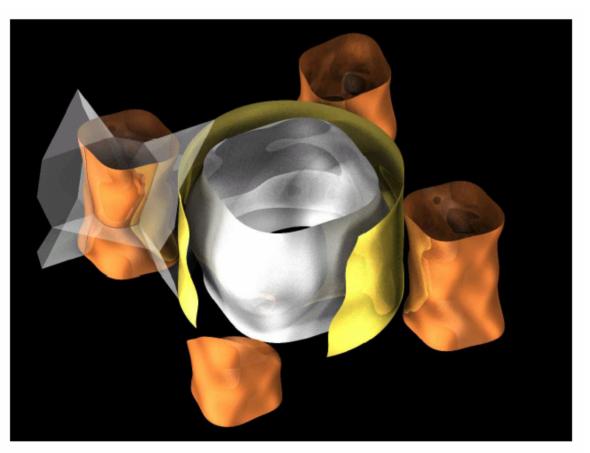
Metals: Fermi Liquid Theory

- Landau: despite (?arbitrarily strong?) interactions—ground state ① filled fermi sea
- Key quantity: position of 'fermi surface' reasonably well calculated by band theory and constrained by 'Luttinger Theorem'
- 'Particles': electrons (with 'renormalized velocity'), plasmons, magnons...(particle-hole pair excitations)....



Sr₂RuO₄: Fermi surface from Quantum Oscillations in Resistivity

C Bergemann et al; Adv Phys. in press



Crucial to Expt:

•Very pure samples

(Y. Maeno)

•High B-Field

Clever Expt

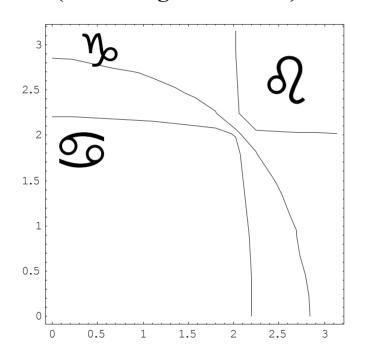
Technique

(Bergemann)

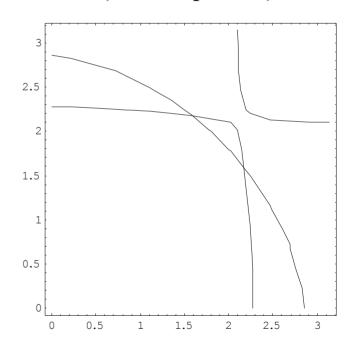
FIG. 28; Visualisation of the Fermi surface of Sr₂RuO₄. The c-sxis corrugation is exaggerated by a factor of 15 for clarity.

Sr₂RuO₄: expt vs band theory

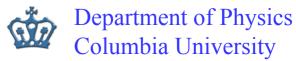
dHvA Fermi surface (from Bergemann data)



LDA Fermi surface (from tb param)



3 sheets. % slightly misplaced in band calc



'Kondo Lattice': carriers vs spins

Basic model for heavy fermion metals....

$$H_{KL} = H_{cond-electron} + J_{Direct} \sum_{\langle i,j \rangle} \overrightarrow{S}_{i} \cdot \overrightarrow{S}_{j}$$
$$+J \int d^{d}r \sum_{spins, i} \delta^{(d)}(\mathbf{r} - \mathbf{R}_{i}) \overrightarrow{S}_{i} \cdot \overrightarrow{\sigma}_{cond-el}(\mathbf{r})$$

Conventional Picture: Spins either

- hybridize into conduction band (fermi surface encloses all electrons)
- •Magnetically order (new periodicity—still
- **'Luttinger theorem)**



Theoretical Possibility: Spins form 'spin liquid'; carriers remain

- •K. A. Kikoin, J. Phys. Cond. Mat. 8 3601 (1996)
- •T. Senthil, S. Sachdev, M. Vojta PRL 90 216403 (2003)

Basic Exptl signature: fermi surface in 'wrong' place More subtle property: topological order

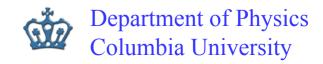
Does this exist in any materials?



Challenges

In dimension d>1, what are the theoretically possible ground states

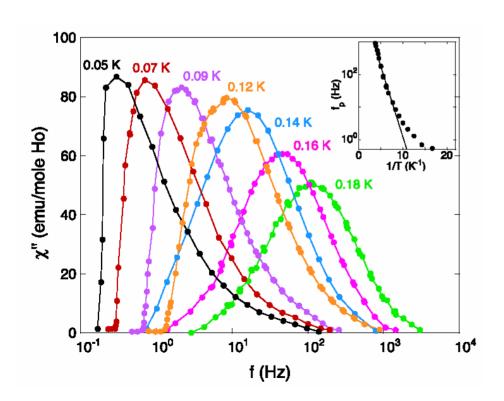
What surprises await, as more materials are explored?



Controlling Quantal Behavior

Ghosh, Parthasarathy, Rosenbaum, Aeppli; Science 296 2195 (2002)

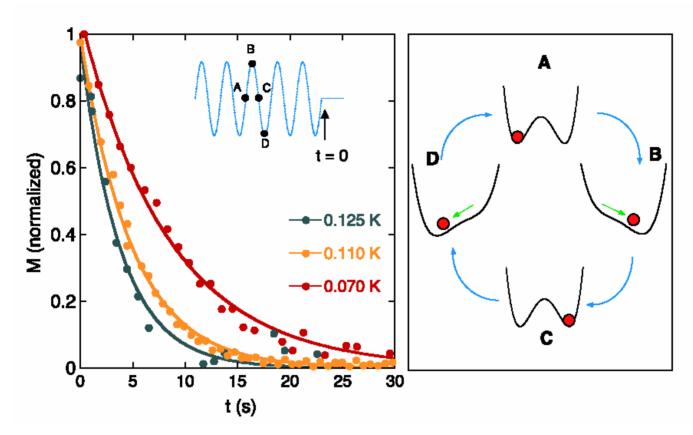
LiHo_{0.045} $Y_{0.955}F_4$: Disordered insulating Ising magnet Interaction: dipolar=>random in dilute system



Distribution of relaxation times narrows on cooling?
—'antiglass behavior'



Long lived spin oscillations

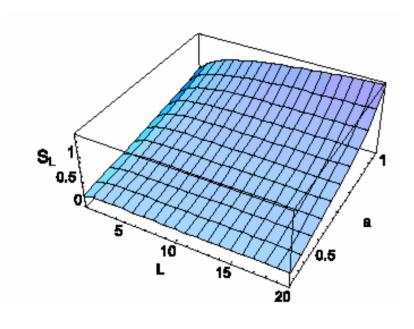


Magnetization induced by 'pump' of given frequency: decay measured in 'rotating frame'. Behavior attributed to coherent precession of multispin cluster (see schematic at left). Message: quantal effects can cause surprising correlated behavior. Question: what is spatial structure? What are correlations?

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Different Instance of Quantal Correlations:

Vidal, Latorre, Rico, Kitaev, quant-phys/0211074



For 1d (but only 1d??) 'Entropy of entanglement' S_L can be shown to diverge at quantum critical point a=1



Challenge

Quantum mechanics + interactions leads to correlations of surprisingly long range in space and time. These are presently inferred from measurements of basically classical quantities.

?How can we measure these more directly?

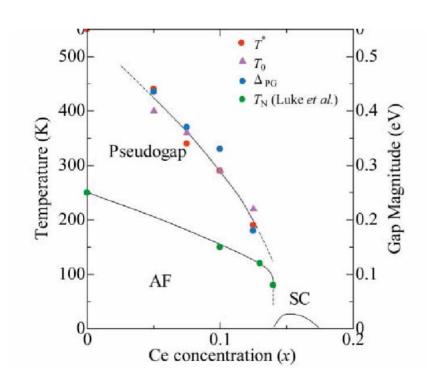
?How can we control and exploit them?



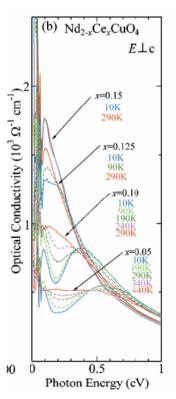
Fluctuations and Material Properties

We all know—long ranged order => gaps

Example: electron-doped high-T_c superconductors



Onose, Taguchi, Ishizawa, Tokura, PRL 87 217001(2001)





But in many materials...

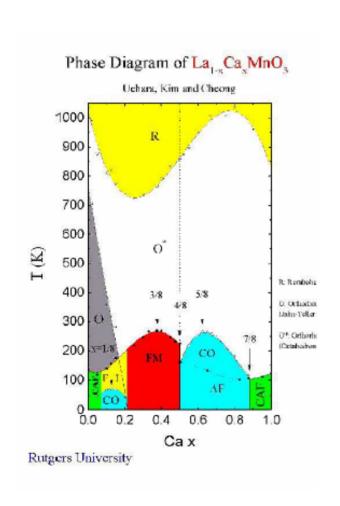
Gap but no (obvious) long ranged order

Probable cause: some kind of short ranged correlations (fluctuating order)

However—although we can 'easily' observe presence of long ranged order, presence and strength of fluctuations harder to determine.

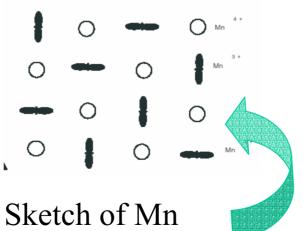


Example: charge and orbital order in 'CMR' materials



'Colossal' magnetoresistance manganites Re_{1-x} Ak_xMnO₃

Many electronic phases, including charge/orbitally ordered insulator

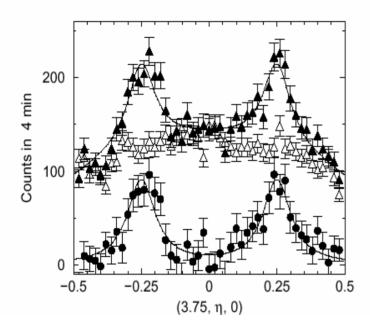


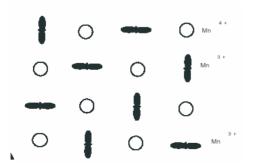
ions in one plane

x=0.5 order note (1/4,0,0) periodicity

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At high T—evidence of short ranged order for x **O**0.5



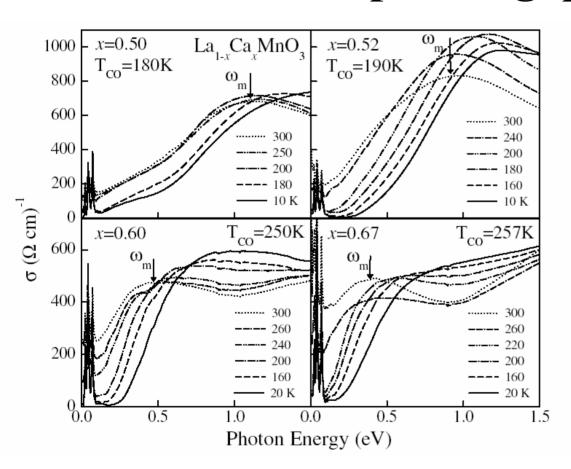


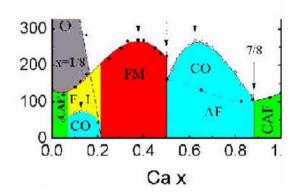
•Neutron scattering: (1/4,0,0) peaks Adams, Lynn, Mukovskii, Aronsov, Shulyatev PRL 85 3954 (2000); x=0.3

Implication: charge modulation strong enough to support orbital order....

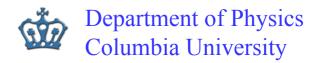


Short range charge order and optical 'pseudogap'



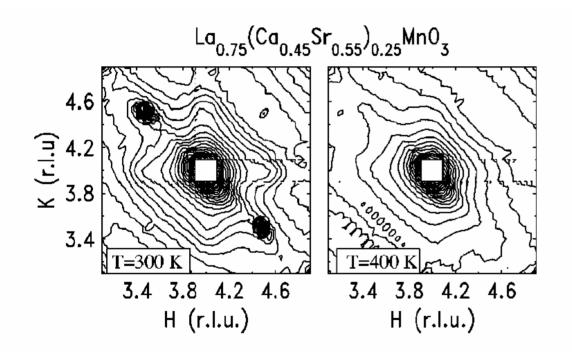


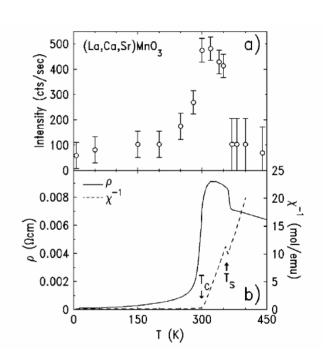
For some compositions, gap persists well above T_{CO} . Natural guess—related to short ranged order. Note: amplitude of flucts not small!



Short ranged order associated with 'pseudogapped' behavior

Kiryukhin, Koo, Ishibashi, Hill, Cheong, PRB67 064421 (2003)





T>380K—no short ranged order.

280<T<380K—short ranged order—bigger □



??intensity??

Estimate of peak intensity relative to bragg peak in long range ordered samples leads to the...

result that the volume fraction of these regions (defined here as the fraction of MnO_6 octahedra experiencing the *correlated* distortion) is smaller than 0.1%. In contrast, a much

?How can such a small scattering intensity lead to such obvious effects on transport/optics??



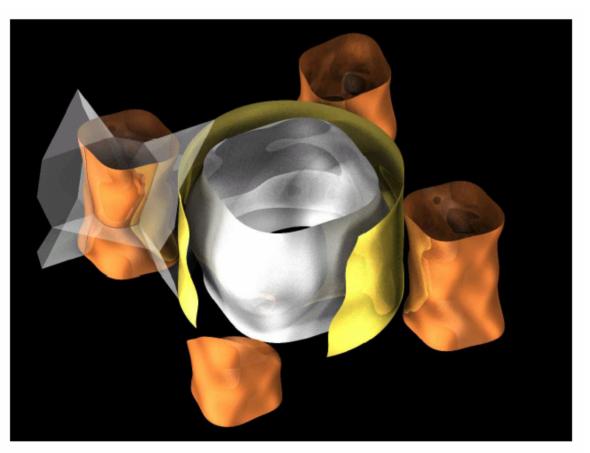
Challenge

How do we detect, normalize and interpret large amplitude fluctuations (in absence of long ranged order)



Sr₂RuO₄: Fermi surface from Quantum Oscillations in Resistivity

C Bergemann et al; Adv Phys. in press



Crucial to Expt:

•Very pure samples

(Y. Maeno)

•High B-Field

Clever Expt

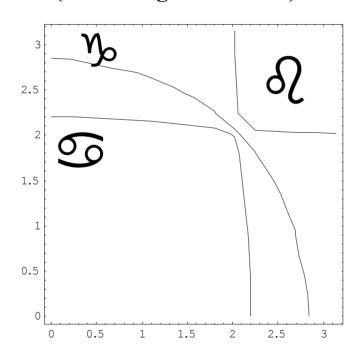
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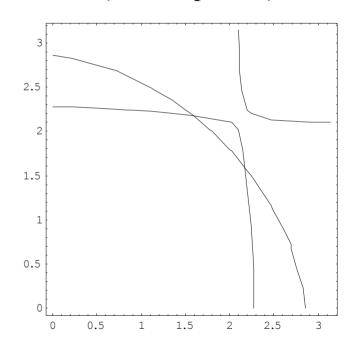
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Sr₂RuO₄: expt vs band theory

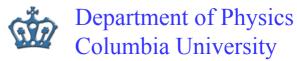
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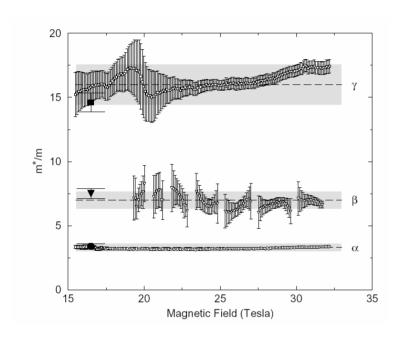
LDA Fermi surface (from tb param)



3 sheets. % slightly misplaced in band calc



Fermi velocity: data vs band theory

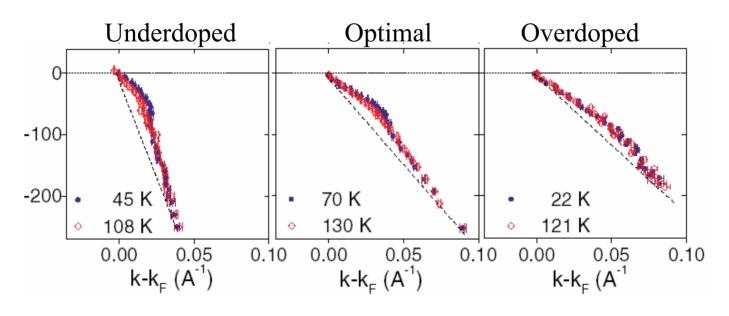


		α	β	γ
Band mass ⁷	m_b/m	1.1	2.0	2.9
Cyclotron mass	m_c/m	2.1	4.3	5.8
Thermodynamic mass	m^{\star}/m	3.3	7.0	16
Susceptibility mass	$m_{ m susc}^{\star}/m$	4.1	8.6	25

Quantum oscillations=>mass == v_F . Conventional band theory underpredicts masses by @3-5x



Other materials—similar story e.g. high T_c



Zone diagonal dispersion => v_F ① 1.8eV-A; weakly doping dependent; roughly indep. of position around fermi surface. Note v_{band} ① 3.8eV-A

Johnson et al PRL87 177007 (2001)



Challenge

Theory of dynamics (electron velocities; linewidths; other correlation functions) with power and utility of density functional based band theory

Tests of the results of this theory??
--More accurate spectroscopies (1-ptcl, 2-ptcl...)



Digression: density functional theory

such that ris minimized at ground state density and value at minimum gives ground state energy

• for tractable and accurate approximation to \mathcal{F}_{univ} (local density approximation and improvements) and convenient procedure for doing minimization (Kohn-Sham equations)



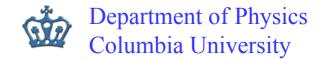
Many-body theory (definitions)

•General Theorem: all many body physics is functional of electron Green function describing propagation of an electron in the lattice potential and interaction field of other electrons

$$G(r,t) = \langle \psi(r,t)\psi^{+}(0,0) \rangle$$

If we restrict attention to the first Brillouin zone then the lattice potential is a matrix in band indices a,b and the effect of interactions in encoded in a self energy which may be spin dependent

$$G_{\alpha\beta}^{ab}(p,\omega) = \left[\omega + \frac{p^2}{2m} + V_{latt}^{ab}(p) - \Sigma_{\alpha b}^{ab}(p,\omega)\right]^{-1}$$



Density functional theory and beyond

•Density functional theory: specific static approx to self energy:

$$G_{\alpha\beta LDA}^{ab}(p,\omega) = \left[\omega + \frac{p^2}{2m} + V_{latt}^{ab}(p) - \Sigma_{\alpha bLDA}^{ab}(p)\right]^{-1}$$

•Full problem: write as DFT (or other approx) + residual (\sim dynamic part of Σ)

$$G_{\alpha\beta}^{ab}(p,\omega) = \left[\omega + H_{LDA}^{ab} - \Sigma_{resid}^{ab}(p,\omega)\right]^{-1}$$

Dynamical Mean Field Method

Metzner/Vollhardt; Mueller Hartmann KOTLIAR

• functional of self energy

minimized at correct self energy and from which ALL RESPONSE FUNCTIONS can be extracted.

• tractable and ?accurate? approximation to $[\{\phi(p, \bullet)\}]$ (local self energy approximation and improvements) and 'convenient' procedure for doing minimization ('quantum impurity model')

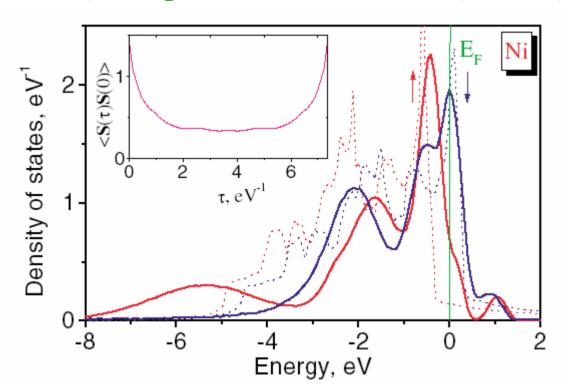
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Main Results so far: local approx

$$(\diamond(p, \diamond) = > \diamond(\diamond))$$

Ex: photoemission DOS for Ni T=0.9T_c (solid lines) compared to LSDA, T=0 (dashed)



Note: side bands (also present at T>T_c) with spin-dependent splitting.

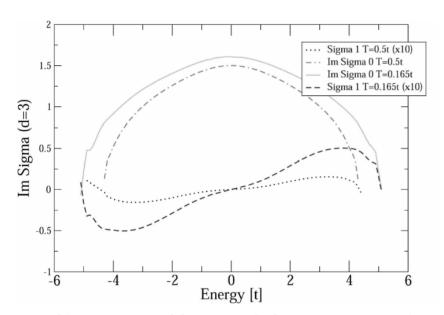
Note: T> behavior (including T_c) predicted no further assumptions.

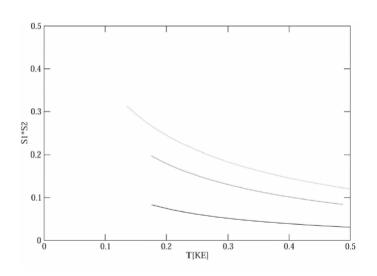
Liechtenstein, Katsnelson, Kotliar PRL 87 067205 (2001).



Directions:

•Momentum dependence (⇔ spatial correlations):

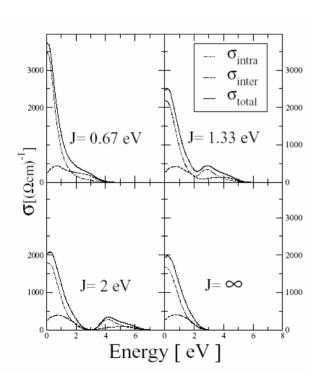




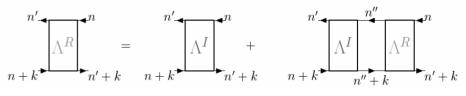
CMR: Effect of further neighbor spin correlations on bandwidth —AJM and H.Monien unpublished

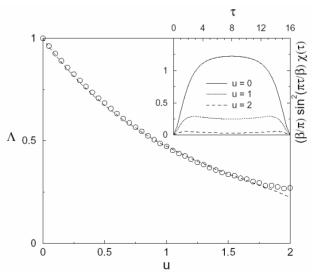
2-particle response functions

Optical conductivity: La_{0.7}Sr_{0.3}MnO₃ T>T_c



Renormalization of dynamical electron-phonon coupling by strong correlations





Challenge:

Experiment vs theory for dynamics:

- •Electron linewidths and velocities
- Conductivity and EELS spectra

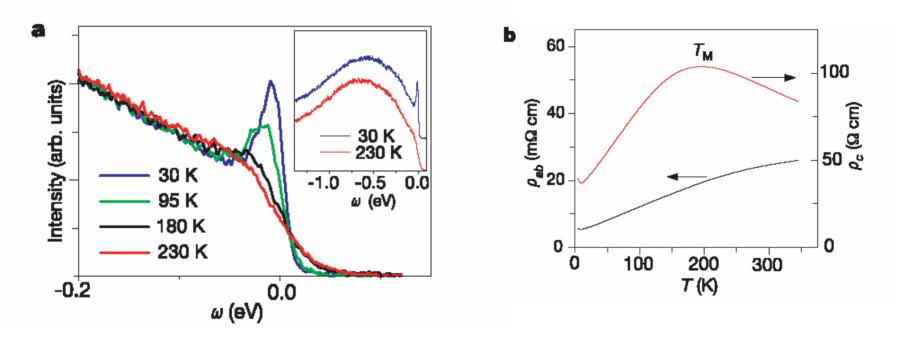
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Transport

•Present understanding: semiclassical theory of electron-like 'quasiparticles' scattering from each other and from phonons

Recent data

Valla, Johnson, Yusof, Wells, Lee, Lourieo, Cava, Mikami, Mori, Yoshimura, Sasaki, Nature **417** p. 627 (2002)



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Presence of quasiparticle correlated with 'metallic' c-axis transport; <u>uncorrelated</u> with ab plane transport in layered 'correlated metal' (Bi/Pb)BaCoO

Surface Science of 'Interesting Materials'

Conventional surface science: key question—where do atoms sit, and why

- •Surface reconstruction (7x7 Si...)
- •Surface structures (steps, islands..)

Correlated electron materials: key question—what is electronic phase and why

- •<u>Electronic reconstruction</u>: different phase at surface
- •Surface electronic structures: locally different phases (nucleated by steps, islands...)

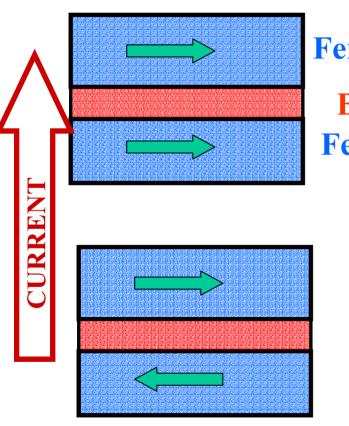


Little studied subject: think of as basic science for potential correlated electron devices

- Device =>interface (more complicated kind of surface)
- •Nanostructure/nanoparticle: in some sense
- 'all surface' (or interface)



'Spin Valve'



Ferromagnet

Barrier

Ferromagnet

Device properties controlled by many body physics (here, magnetism) at the interface

Parallel spin: more current

Antiparallel spin: less current



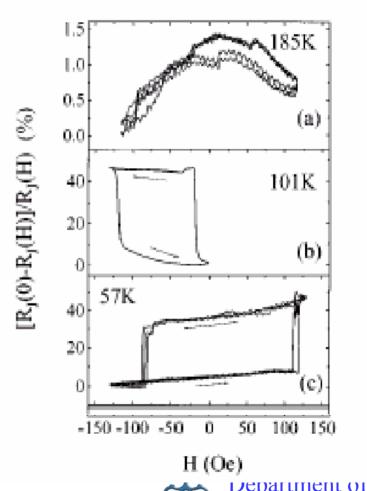
CMR Spin valve

(J. Sun, IBM)

Spin valve based on La_{0.7} Sr_{0.3}MnO₃ T_c bulk=380K.

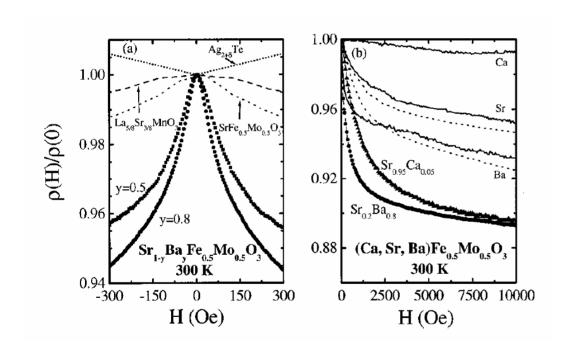
Device dies by $T = T_c/2$

=>Something happens at interface



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'Tunneling Magnetoresistance'



Large room temperature magnetoresistance in ceramic sample attributed to antiferromagnetic layers on surface of grain

Kim, Hor, Cheong, APL 79 368 (2001)



Challenge

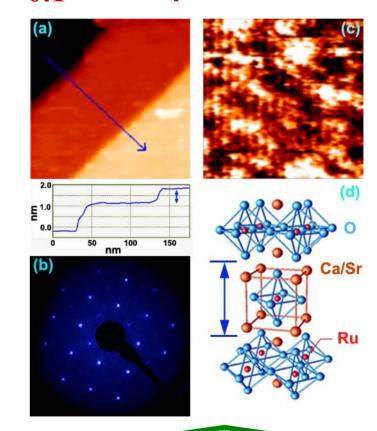
What is going on at the interface?? Is there a new phase at low T?? Does one appear as T is raised??



Different electronic phase at the surface: Ca_{1.9}Sr_{0.1}RuO₄

Bulk metal insulator transition at T=150K but surface stays metallic to T=125K

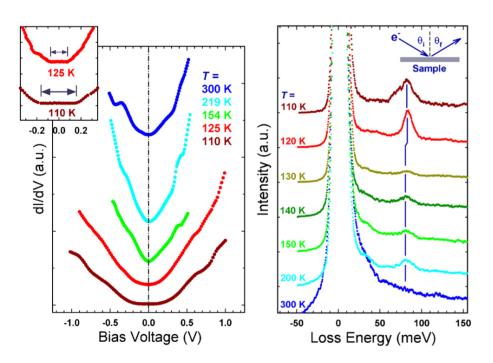
J. Zhang, D. Mandrus, E. W. Plummer ORNL

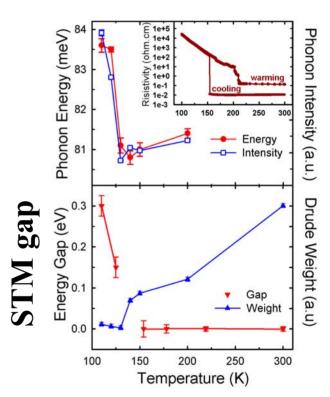


Basic surface science (Topography STM atomic resolution, LEED)



Surface remains metallic to lower T!



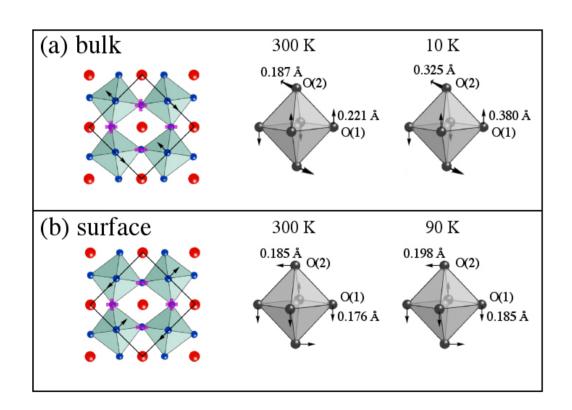


IV: gap opens at 125K (bulk transition 150K)

EELS—phonon turns on at transition (bulk seen weakly; surface strongly)

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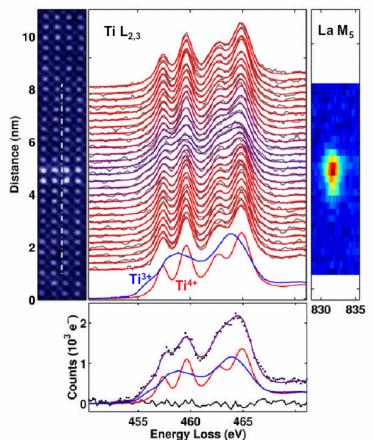
Proposed Mechanism

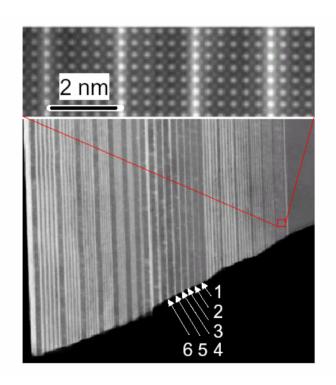


Different structure at surface (bond length; magnitude and direction of RuO₆ tilts increases hopping; favors metallic phase.



Interface—correlated (LaTiO₃) and uncorrelated (SrTiO₃) material

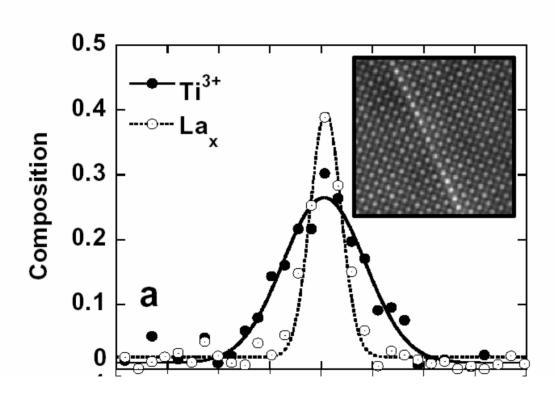




Ohmoto, Muller, Grazul and Hwang.



Charge variation across interface—from TEM/ EELS



Charge profile: one monolayer of La



Challenge

Surface/interface science of correlated materials: electronic surface reconstructions.
What are they? How do you see them? What are their properties?



Summary

- 'Correlated electron materials science' is a "frontier field"-we don't know what we are going to find=>exploratory research—more and higher quality materials
- •Quantal correlation/entanglement—how do you see it? How do you exploit it?
- •Dynamics (electron spectral function; conductivity; density-density correlation) on same level as DFT ground state—coming within our grasp
- •Surface/interface science of electronically active materials!!

